The Use of Microporous Metal-Organic Frameworks for the Storage of Oxygen

Jared B. DeCoste,[1] Mitchell H. Weston,[2] Patrick E. Fuller,[2] Trenton M. Tovar,[3] Gregory W. Peterson,[1] M. Douglas LeVan,[3] and Omar K. Farha[2]

[1]Edgewood Chemical Biological Center, Aberdeen Proving Ground, MD, [2] NuMat Technologies, Skokie, IL, [3] Vanderbilt University, Nashville, TN

Relevance

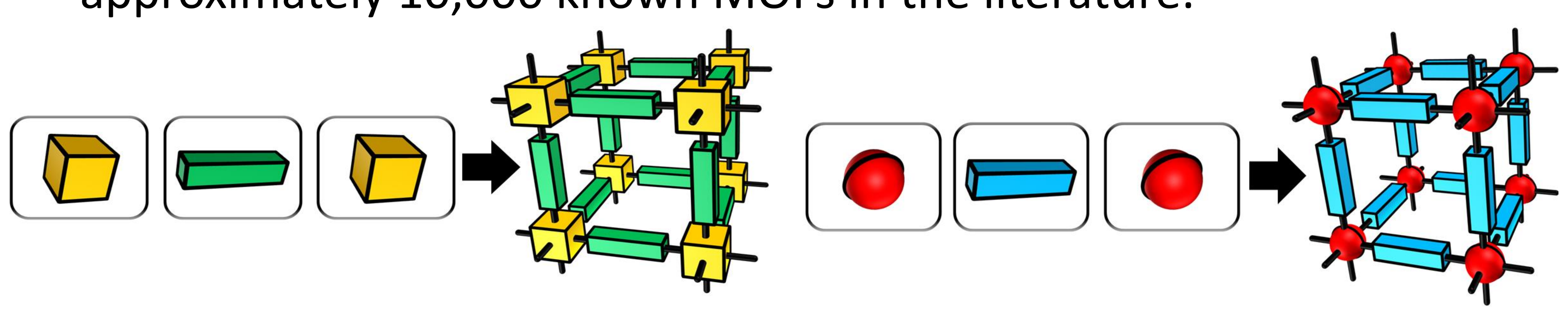
In certain situations, where a gas mask would not suffice, the warfighter may need a fresh oxygen supply. For instance:

- Emergency oxygen for airplanes
- Medical oxygen on the battlefield
- Special Operations
- High concentration/unknown chem/bio threats
- Fires where the oxygen concentration is diminished
- Emergency oxygen for underground/hardened facilities

Maximizing the amount of oxygen a given volume can hold at a given pressure is important. An adsorbent that can substantially increase the amount of oxygen could allow for the development of lower pressure storage systems such as a conformal backpack.

Metal-Organic Frameworks

Metal-organic frameworks (MOFs) in their most rudimentary form are metal/metal-oxide nodes connected together by organic linkers to form a repeating 3-dimensional structure. In many cases this structure has pores that can be tailored in size and chemical functionality. Due to the potentially infinite number of metal and linker combinations, there are approximately 10,000 known MOFs in the literature.



As adsorbents MOFs are ideal because of the following characteristics:

- Simple synthesis
- Modular building blocks that can be interchanged given a large number of materials with various properties.
- High crystallinity allows for computational modelling
- Enormous internal surface areas up to 7,200 $m^2 g^{-1}$

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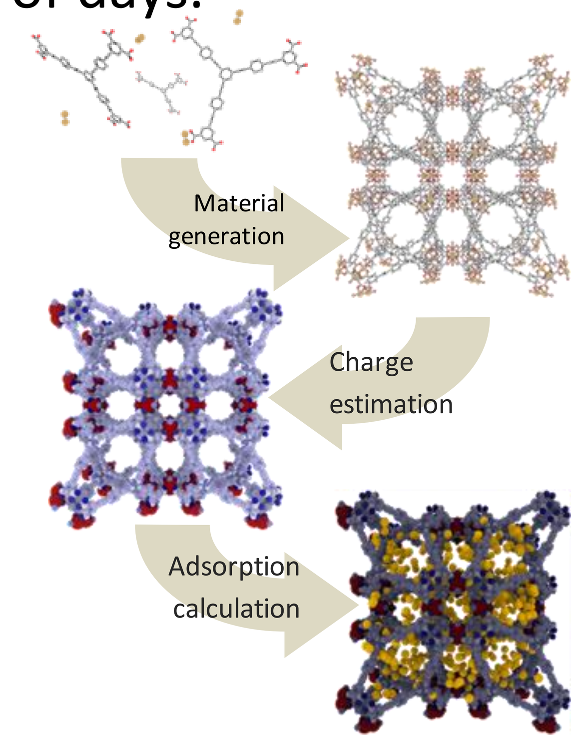
Computational Screening

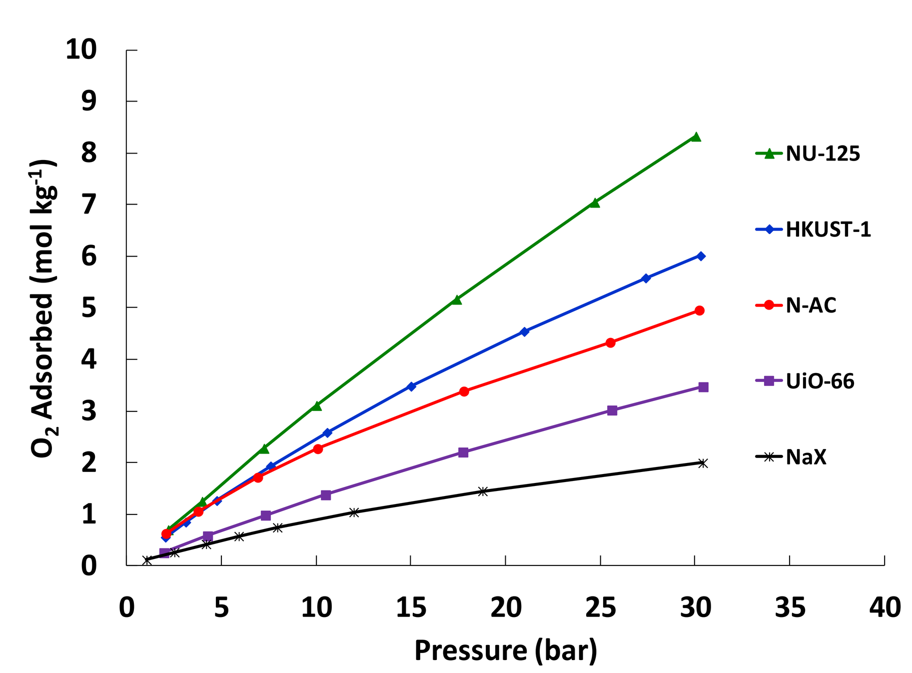
Studying the oxygen uptake on every known MOF would be impossible. However, Grand Canonical Monte Carlo simulations (GCMC) allowed us to simulate the oxygen uptake of approximately 10,000 MOFs in the matter of days.

- First, a series of MOFs was generated and geometries optimized.
- A charging algorithm was applied to each MOF
- An oxygen adsorption isotherm was calculated for each MOF
- The most promising MOFs were selected for experimental studies

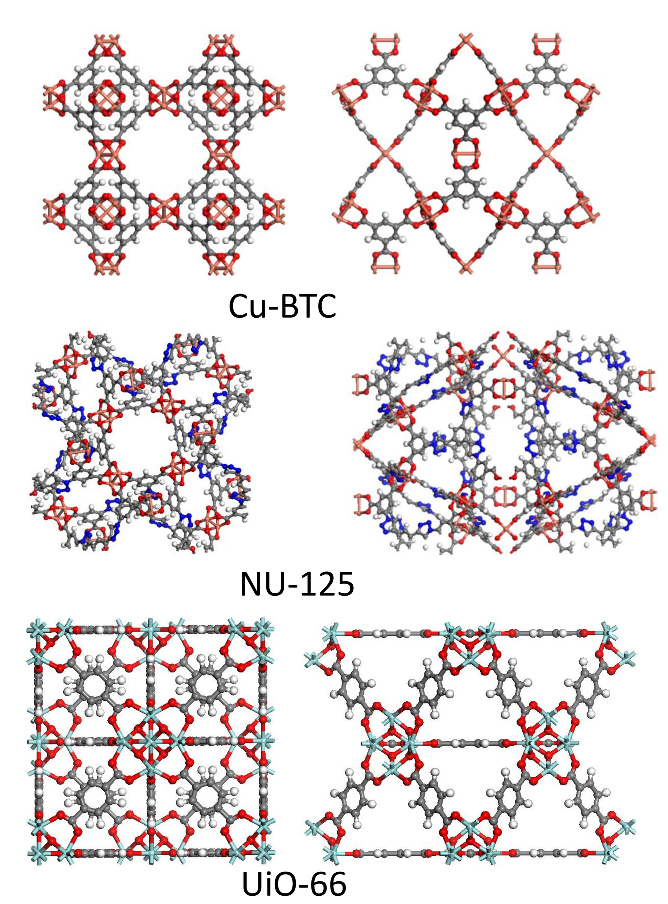


Experimental Oxygen Uptake

Two MOFs, HKUST-1 and NU-125, both copper based MOFs, were selected as the most promising candidates for oxygen adsorption and studied further. Their uptakes were compared to UiO-66, a zirconium based MOF known for its high stability, Norit SX Ultra (N-AC), an activated carbon with high surface area, and NaX, a zeolite that is the current state of the art used by many for oxygen uptake.

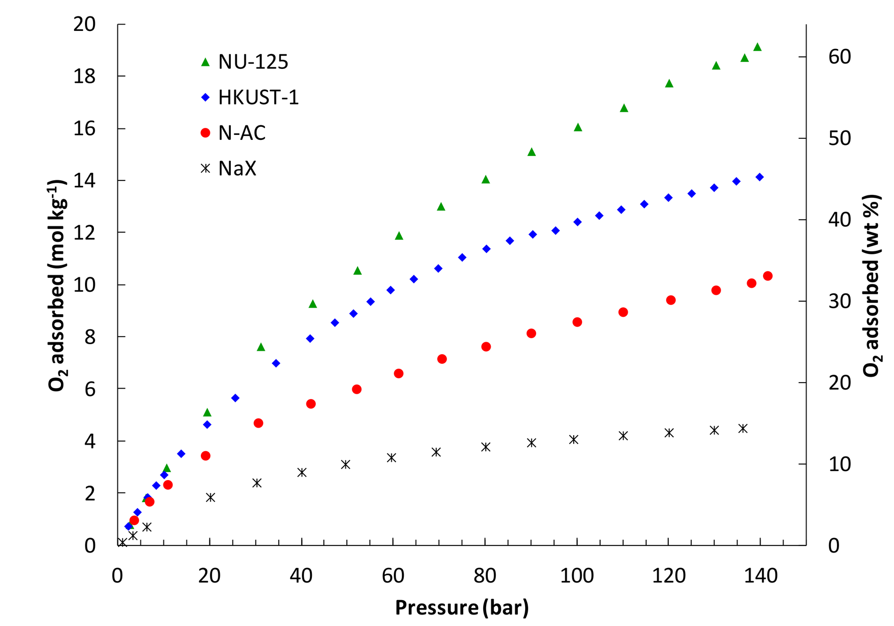


Excess oxygen isotherms measured at 298K up to 30 bar



High Pressure Uptake

- Materials were examined up to 140 bar (2030 psi), the standard operating pressure of an oxygen cylinder.
- HKUST-1 and NU-125 were able to adsorb and release oxygen over 50 cycles with no loss in capacity.

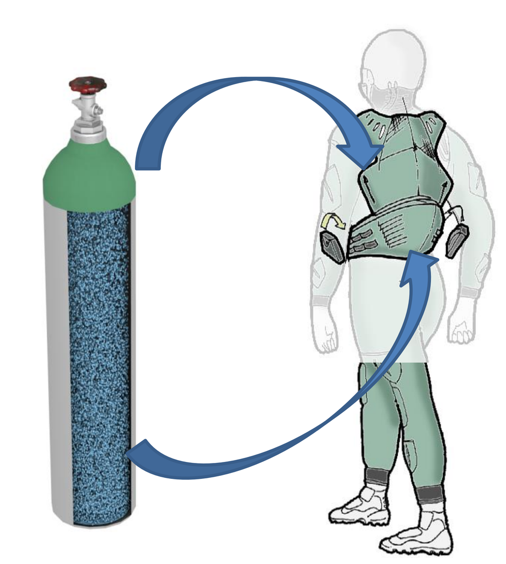


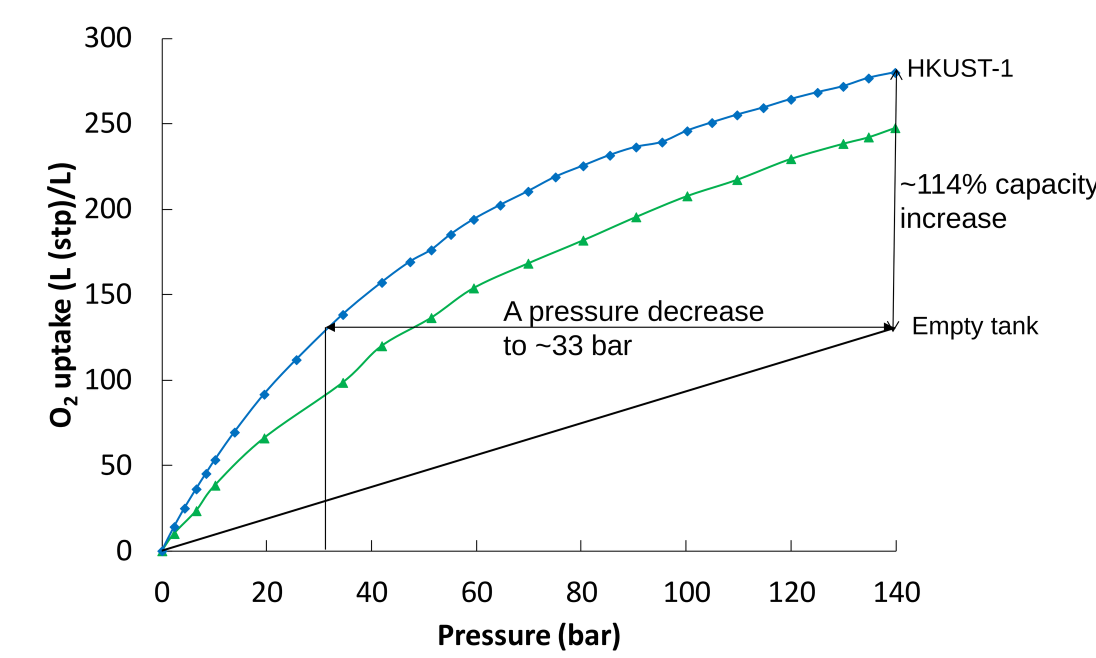
Absolute oxygen isotherms measured at RT up to 140 bar

The Warfighter Impact

Verse an empty tank, one filled with HKUST-1 would have the following potential benefits:

- Doubling the capacity, extending the length of a potential mission, or decreasing the size of the tank needed.
- The same capacity could be achieved at a pressure of ~33 bar (480 psi), allowing the use of containers that are not as bulky, and potentially conformal to the body.





Absolute oxygen isotherms measured at RT on a per volume basis

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